NEW COMPLEX BASIS FUNCTIONS FOR VARIATIONAL CALCULATION COULOMB SYSTEMS

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Early [1] was proposed new types of basis functions for variational calculations of the quantum-mechanical systems with Coulomb interaction between the particles. This is complex exponential functions are depended by all inter-particles distances. On calculations of various three particle systems was shown that a single complex exponential basis function can replace from 10 to 15 real exponential functions in calculations ground state of atom like systems and up to 80 such functions in case molecular-like systems. It is necessary to underline, that calculation formulas for matrix elements of a energy operator with complex exponential functions are very simple for three particle system, but are complicated for four particle systems [2], and unknown for many particle systems. That creates calculation problems for using such functions for many particle systems. For avoiding this problem is proposed to use complex Gaussian functions, depending by all inter-particle distances. Calculations with these functions are simple by using complex numbers arithmetic. For testing new functions we carry out variational calculations with that basis (45 complex functions) for same four particle systems, such as positronium molecule, molecular hydrogen, tritium, deuterium. For example, we obtain binding energy equal to -0.513 atomic units for positronium molecules. Sufficiently close results obtain for other systems. Our results show that new basis functions alike complex exponential functions can be significantly improve the accuracy of variational calculations for Coulomb systems with taking account correlation and adiabatic effects.

[1] T. K. Rebane and O. N. Yusupov, Zh. Eksp. Teor. Fiz. **98**, 1870 (1990).
[2] V. S. Zotev and T. K. Rebane, Phys. Rev. A **65**, 062501 (2002).